An efficient Monte Carlo algorithm for the evaluation of Renyi entanglement entropy of a general quantum dimer model at the R-K point

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A highly efficient and simple to implement Monte Carlo algorithm is proposed for the evaluation of the Renyi entanglement entropy(REE) of quantum dimer model(QDM) at the Rokhsar-Kivelson(R-K) point. It makes possible the evaluation of REE at the R-K point to the thermodynamic limit for a general QDM. We apply the algorithm to QDM on both triangular and square lattice as demonstrations and find the REE on both lattices follow perfect linear scaling in the thermodynamic limit, apart from an even-odd oscillation in the latter case. We also evaluate the topological entanglement entropy(TEE) on both lattices with a subtraction procedure. While the expected TEE of $\ln 2$ is clearly demonstrated for QDM on triangular lattice, a strong oscillation of the result is found for QDM on square lattice, which implies the relevance of boundary perturbation in such a critical system.

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I. INTRODUCTION

Spin liquid phases in quantum magnet[1] are exotic state of matter that can realize novel quantum structures. The topological order is one of such possibility. The topological order manifests itself in both the nontrivial ground state degeneracy on multiply connected manifold, and the topological contribution to the entanglement entropy.

The quantum dimer model(QDM) is the simplest model system to illustrate the spin liquid physics[2, 3]. In a QDM, the basic degree of freedom is the dimer living on the bonds of the lattice. Each site of the lattice should be involved in one and only one dimer. A dimer can be viewed as a spin singlet pair in the resonating valence bond theory and can hop from bond to bond through the kinetic term of QDM. At the so called the Rokhsar-Kivelson(R-K) point, the ground state of QDM becomes the equal amplitude superposition of all the allowed dimer coverings of the lattice. Such a state can be viewed as a spin liquid if we interpret a dimer as a spin singlet pair.

On multiply connected manifold, the Hilbert space of QDM factorizes into distinct topological sectors that can not be connected by any local Hamiltonian term to any finite order. As an example, for QDM defined on a two dimensional torus, we can introduce two reference lines around each of the two holes of the torus and classify a dimer configuration into one of four sectors according to the parity of the number of dimers that cross the two reference lines in this configuration. It is clear that such parities are conserved by any local Hamiltonian term and thus the Hilbert space factorizes into four disconnected pieces. Since the different sectors are locally indistinguishable, any local Hamiltonian defined on such factorized Hilbert space should exhibit at least four-fold degeneracy. The existence of such locally indistinguishable, but globally distinct degenerate states on multiply connected manifold is one important signature of a topological ordered state.

On bipartite lattice, additional subtlety emerges. Rather than the parity of the crossing numbers, an integer-valued quantity is conserved by all local Hamiltonian terms. As a result of such a subtle difference, the QDM defined on frustrated and on unfrustrated lattice have distinct properties. For example, while the QDM on the triangular lattice has a short-ranged dimer correlation and exhibits well defined Z_2 topological order at the R-K point[3, 4], the QDM at the R-K point on the square lattice actually corresponds to a critical system with algebraic dimer-dimer correlation and no topological order.

The topological entanglement entropy(TEE) is recently proposed as another way to characterize a topological ordered system[5, 6]. Unlike topological degeneracy, TEE can be measured directly in the ground state wave function with no reference to the excitation spectrum. For a gapped system, the entanglement entropy generally satisfies the so called area law, $S = \alpha A - \gamma$, in which A is the area of the boundary separating the subsystem from the environment. What makes a trivial short range correlated state different from a topological ordered state is that the latter exhibits a nonzero universal topological contribution γ to the entanglement entropy.

Besides being a useful way to characterize the topological order, the information contained in the entanglement entropy can be used more generally to diagnose the correlation in the system. In critical system, correction to the linear scaling of entanglement entropy is also generally expected[7–13]. From such corrections, important information about the low energy physics of the system can be extracted.

For both of these purposes, an efficient algorithm is needed for the evaluation of the entanglement entropy of

QDM on large enough subsystem. In the evaluation of entanglement entropy, the central task is to enumerate the number of the dimer configurations in the subsystem that is compatible with the fixed dimer configuration on the boundary with the environment. For QDM defined on planar graph, this can be done with a Fermioic representation of the dimer degree of freedom[14–16]. However, as the number of dimer configurations on the boundary grows exponentially with the size of the subsystem, such an algorithm is exponentially expensive for large subsystem(see [16] for an exception in the special geometry of an infinite cylinder). For non-planar lattice such as three dimensional lattice, no efficient algorithm is known to enumerate the dimer covering number.

For these reasons, the evaluation of TEE of QDM is limited to subsystem of rather small size. As a result, the confirmation of the $\ln 2$ TEE for QDM on triangular lattice is still subjected to rather large finite size uncertainty[4]. The situation become even worse for QDM on square lattice, for which the dimer correlation is long-ranged and finite size effect is much stronger. Furthermore, for QDM on 3D lattice and nonplanar 2D lattice, which are of great theoretical interest, almost no result exist.

Thus, it is highly desirable to develop an efficient and easy to implement algorithm to evaluate the entanglement entropy of a general QDM at the R-K point. This is possible with the Monte Carlo sampling, as the problem reduces to a classical statistical problem at the R-K point. However, as the quantity to be averaged suffers from an exponentially growing fluctuation with the growth of the subsystem size, which is just the origin of the area law for entanglement entropy, the convergence of the result becomes exponentially slow.

In this paper, a re-weighting trick is proposed to overcome this difficulty, which makes possible the evaluation of Renyi entanglement entropy of general QDM at the R-K point to the thermodynamic limit. We apply this algorithm to QDM on both the square and the triangular lattice. We focus on two issues, namely the scaling form of REE and the topological contribution TEE. We find while the REE follows perfect linear scaling on triangular lattice, a robust even-odd oscillation with the subsystem size in REE is observed for QDM on square lattice. Nevertheless, we find the REE for even and odd sized subsystem still follows perfect linear scaling. We find the TEE on triangular lattice converge quickly to the expected value of $\ln 2$ with increasing subsystem size, while that for square lattice exhibit strong oscillation and does not converge.

This paper is organized as follows. In the next section, we describe the way to evaluate the entanglement entropy with Monte Carlo sampling in QDM. We also point out the origin of difficulty with the conventional algorithm and introduce the re-weighting trick to solve such difficulty. In section III, we demonstrate the new algorithm with two examples, namely the QDM on square lattice and triangular lattice, and present results on both the scaling form of REE and the value of the topological contribution TEE calculated from a subtraction procedure. In section IV, we present a discussion on the result obtained and some outlook on the application of the new algorithm to more general QDM.

II. THE RENYI ENTANGLEMENT ENTROPY OF QDM

The ground state of a general QDM at the R-K point has the following form

$$|\Psi\rangle = \sum_C |C\rangle. \tag{1}$$

Here $|C\rangle$ denotes a general dimer covering of the lattice in a specific topological sector. Each lattice site should be involved in one and only one dimer in this covering.

To characterize the entanglement property of the system, we divide it into two parts: a subsystem and the corresponding environment that meet at their common boundary. The reduced density matrix of the subsystem is then given by tracing out the degree of freedom in the environment from the density matrix of the system

$$\rho_s = Tr_e |\Psi\rangle\langle\Psi| \tag{2}$$

and the entanglement entropy of the Von Neumann type is defined as

$$S_{\rm vN} = -Tr\rho_s \ln \rho_s. \tag{3}$$

However, it is in general quite hard to evaluate the Von Neumann entropy numerically from this definition. A quantity that is much easier to evaluate is the Renyi entropy. The Renyi entropy of order n is given by

$$S_n = -\frac{1}{n-1} \ln Tr\rho_s^n. \tag{4}$$

The Von Neumann entropy is related to the Renyi entropy by $S_{\rm vN} = \lim_{n\to 1} S_n$ and the two entropies share many common properties in the long wave length limit. In particular, it is found that the universal topological contribution γ extracted from S_n is independent of the value of n and agree with the value extracted from $S_{\rm vN}$[17].

In the following, we will focus on the evaluation of S_2, although the algorithm proposed below can be readily generalized to evaluate S_n with $n > 2$. To evaluate S_2, we use the replica trick[18, 19] and introduce an identical copy of the system as its replica, which is divided in exactly the same manner as the system into a subsystem and the corresponding environment. The state vector of the whole system is then given by the direct product of

the state vector of the two copies, $|\Psi \otimes \Psi\rangle$. It can be shown that

$$Tr\rho_s^2 = \langle \Psi \otimes \Psi | \widehat{\mathrm{SWAP}} | \Psi \otimes \Psi \rangle, \tag{5}$$

in which $\widehat{\mathrm{SWAP}}$ denotes the operation of exchanging all the degree of freedoms within the subsystem between the system and its replica[18]. As the degree of freedom of a QDM is defined on the bonds of the lattice, one should be careful about the partition of the degree of freedoms. In Fig.1, a partition on the square lattice is shown. In this partition, all bonds whose midpoint that lie within the boundary line is defined to be degree of freedom in the subsystem. Otherwise it is defined to be degree of freedom of the environment.

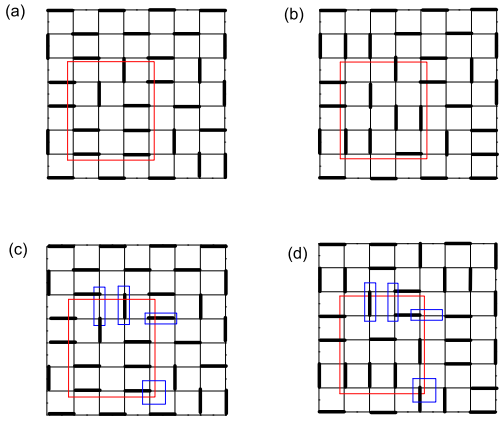

FIG. 1: Upper panel: an illustration of the partition of degree of freedom and an example of swappable dimer configuration of the system(a) and its replica(b). The subsystem is defined to be the region within the red boundary lines. The dimers are shown with the thick links. Lower panel: an example of non-swappable dimer configuration of the system(c) and its replica(d). The locations of local violation of the dimer constraint in the swapped configuration are highlighted by the blue frames. In this example, $N_{err} = 4$.

With such a partition, $Tr\rho_s^2$ can be represented in the following form that is directly accessible to Monte Carlo sampling

$$Tr\rho_s^2 = \frac{\sum_{C_1,C_2} S(C_1,C_2)}{\sum_{C_1,C_2}}. \tag{6}$$

Here the summation is over all the dimer configurations in the system (C_1) and its replica (C_2). $S(C_1,C_2)$ equals to one if the swaped configuration still satisfy the dimer constraint in both the system and its replica and is zero otherwise. An example of swappable dimer configuration is shown in Fig.1a and 1b. A close inspection shows that C_1 and C_2 is swappable only when the following two conditions are met. First, on each bond in the subsystem that cross the boundary line, the dimer occupation number in the system and its replica must be the same. Second, on those bonds that cross the boundary line but belong to the environment, the total number of dimers on those bonds that terminating on the same site in the subsystem must be the same for the system and its replica. Obviously, the number of such local constraint grows linearly with the length of the boundary line. As a result, the probability for two independent dimer configurations C_1 and C_2 to be swappable decreases exponentially with the length of the boundary. This is just the origin of the area law, and it at the same time make clear the difficulty of evaluating the entanglement entropy with Monte Carlo sampling, which amounts to averaging a quantity with an exponentially large fluctuation.

However, the difficulty with the exponentially increasing fluctuation in the sampling of entanglement entropy can be solved by the following re-weighting trick. First, we re-write the sum in Eq.(6) in the following form

$$Tr\rho_s^2 = \frac{\sum_{C_1,C_2}(r_0)^{N_{err}}}{\sum_{C_1,C_2}(r_1)^{N_{err}}}. \tag{7}$$

Here $r_0 = 0$ and $r_1 = 1$, N_{err} is the number of times that the local dimer constraint is violated in the swaped configuration(See Fig.1c and 1d for a detailed illustration of the meaning of N_{err}). It is then clear that the large fluctuation in sampling $Tr\rho_s^2$ originates from the huge difference in the distribution that appear in the denominator and the numerator. A simple solution to this problem is to introduce a sequence of intermediate values r_i and rewrite the quantity in term of the product of a serials of ratios,

$$Tr\rho_s^2 = \prod_{i=1,m} \frac{\sum_{C_1,C_2}(r_{i-1})^{N_{err}}}{\sum_{C_1,C_2}(r_i)^{N_{err}}}, \tag{8}$$

in which $r_0 = 0$, $r_m = 1$ and $r_i < r_j$ for all $i < j$. If the difference between the successive r_i is chosen to be sufficiently small, then each term in the product can be simulated efficiently. In practice, we have divided the region $[0,1]$ into 10 equal intervals, which is found to be fine enough for good convergence for subsystem with size up to 16×16, which is already quite large. For even larger subsystem, one should introduce more intervals. However, since the number of intervals needed only scales linearly with the subsystem size, the thermodynamic limit can be easily approached.

III. APPLICATION OF THE NEW ALGORITHM

A. Scaling form of the Renyi entanglement entropy

We apply the above algorithm to evaluate the Renyi entanglement entropy of QDM at the R-K point on both triangular and square lattice. The big system is defined

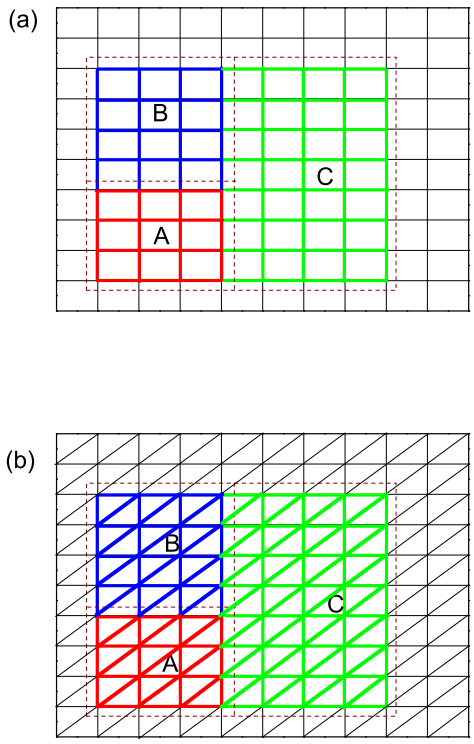

FIG. 2: The partition of the dimer degree of freedoms on the lattice used to evaluate REE and TEE on (a) square lattice, (b)triangular lattice. The subsystem used in the evaluation of REE are all of A-type, for which all bonds that cross the boundary are defined to be degree of freedom in the environment. The three subsystems A, B and C separated by the dashed boundary lines will be used later to extract the TEE. In this partition, a bond belongs to a given subsystem when its midpoint belongs to that subsystem. Thus all bonds in red belong to subsystem A, all bonds in blue belong to subsystem B and all bonds in green belong to subsystem C. The remaining bonds all belong to the environment. Note that although subsystem A and B contains the same number of sites, they have different number of bonds.

on a torus with a fixed size of 30×30 sites and the subsystem is chosen to contain $n_a \times n_a$ lattice sites with $2 \leq n_a \leq 16$. An illustration of the subsystem is given in Fig.2. All bonds that cross the boundary line are defined to be degree of freedom in the environment in this calculation. We use $L = 4n_a$ as a measure of the boundary length. Note such a definition of boundary length has an inherent ambiguity on a lattice.

The Renyi entanglement entropy S_2 of QDM on both the triangular and the square lattice are shown in Fig.3. The error bar is smaller than the symbol size. For the triangular lattice, a rather good linear scaling of S_2 with n_a is observed starting from a rather small value of $n_a = 2$, which is consistent with the short ranged nature of the dimer correlation in the QDM on triangular lattice. The Renyi entropy S_2 can thus be fitted well by the following form

$$S_2 = \alpha L - \beta. \tag{9}$$

Note as a result of the ambiguity in the definition of the boundary length, β can not be directly interpreted as the topological contribution to the entanglement entropy. The fitted values are $\alpha = 0.585$ and $\beta = 2.85$.

For the square lattice, the result is markedly different. As can be seen in Fig.3b, an even-odd oscillation in the Renyi entanglement entropy is observed. Such an oscillation is also reported in other recent studies of QDM and spinful short range RVB state on square lattices and is attributed to the critical nature of the QDM on the unfrustrated square lattice, which results in the relevance of the boundary perturbation on S_n for n greater some critical value[16]. For QDM on square lattice, it is found that $n_c < 2$. Thus S_2 is already susceptible to boundary perturbation.

However, if we plot S_2 separately for subsystem with an even and odd n_a, as is shown in Fig.4, it is clear that both results follow perfect linear scaling for large n_a,

$$\begin{aligned} S_2^e &= \alpha_e L - \beta_e \\ S_2^o &= \alpha_o L - \beta_o, \end{aligned} \tag{10}$$

where the offset β_e and β_o are found to be negligible. It is also seen that the linear scaling starts at a much larger value of $n_a = 6$ than that on triangular lattice. This is consistent with the fact that the QDM on square lattice has a long-ranged dimer correlation.

B. Topological entanglement entropy

We now turn to the evaluation of TEE. For this purpose, we divide the subsystem into three parts, A, B and C. Both A and B contain $n_a \times n_a$ sites and C contains $n_a \times 2n_a$ sites. Then the topological contribution to the entanglement entropy can be extracted by subtracting out all the non-universal contributions with the following combination

$$-\gamma = S_2^A + S_2^B + S_2^C - S_2^{AB} - S_2^{AC} - S_2^{BC} + S_2^{ABC}. \tag{11}$$

Different from the spin system, care must be paid on the partition of the dimer degree of freedom into the subsystems. For this purpose, in Fig.2 we have plotted the bonds of different subsystems with different colors. As a result of the difference in the assignment of boundary degree of freedom, $S_2^A \neq S_2^B$ and $S_2^{AB} \neq S_2^C$. Thus, all the seven terms in Eq. 11 should now be calculated independently[19].

We will first present the result of TEE for QDM on triangular lattice, which is expected to show robust topological order and a TEE of $\gamma = \ln 2$[3, 4]. This is confirmed

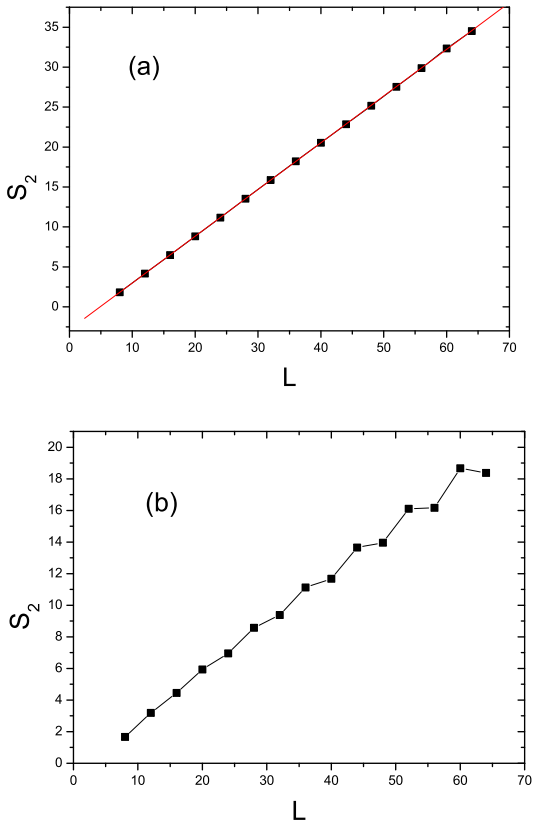

FIG. 3: The Renyi entanglement entropy S_2 of QDM as a function of the boundary length $L = 4n_a$. (a)triangular lattice, (b)square lattice. The thin lines are guide to the eyes.

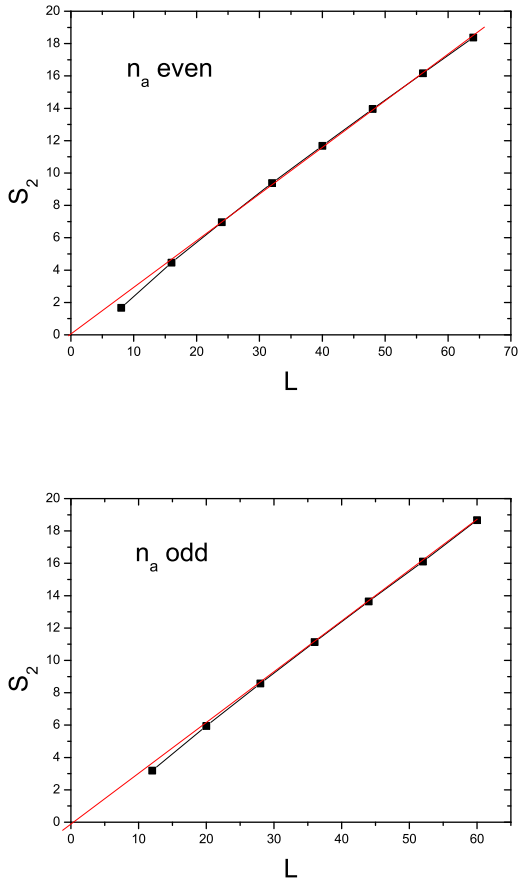

FIG. 4: The Renyi entanglement entropy S_2 of QDM on square lattice as a function of the boundary length $L = 4n_a$ for even(a) and odd(b) n_a. The thin lines are guide to the eyes.

by our calculation. As is shown in Fig.5a, in which the TEE is plotted as a function of n_a, γ converges steadily to the expected value of $\ln 2$. Since the QDM on triangular lattice has a rather short-ranged dimer correlation, we expect γ to converge to its thermodynamical limit at small n_a. From the result it is also clear that the value extracted from linear extrapolation of $S_2(\beta = 2.85)$ can not be interpret as the TEE and it is important to to perform the subtraction procedure as indicated in Eq. 11 to remove the ambiguity in the definition of the boundary length.

For the square lattice, the situation is quite different. As shown in Fig.5b, the topological contribution extracted from Eq.11 exhibits strong oscillation with n_a and never converge. This is consistent with our understanding that the R-K point of the QDM on square lattice describe a critical system, for which the topological order is unstable. The strong oscillation is the result the even-odd effect mentioned above, which implies again the relevance of the boundary perturbation in such a critical system.

IV. DISCUSSIONS

In this paper, we have presented a very efficient and simple to implement Monte Carlo algorithm for the evaluation of the Renyi entanglement entropy of QDM at the R-K point. The algorithm is general and simple enough that it can be easily implemented for QDM defined on a general lattice. A generalization of the algorithm for S_n with a higher order n is also straightforward.

As a demonstration of the new algorithm, we have applied it to the QDM defined on triangular and square lattice. On triangular lattice, the $\ln 2$ TEE and the perfect linear scaling of REE in the thermodynamic limit, which are expected from effective theory arguments, are clearly demonstrated. On the other hand, an interesting even-odd oscillation in REE is observed for QDM on square lattice, which agrees with previous studies and implies the relevance of boundary perturbation in such a critical system. However, even if the dimer correlation is long

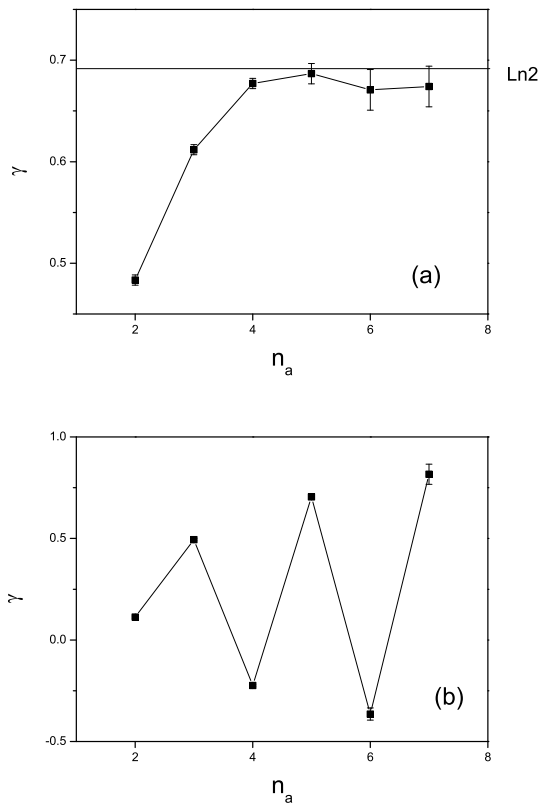

FIG. 5: The topological entanglement entropy extracted from Eq. 11 for QDM on triangular(a) and square(b) lattice. The thin lines are gude to the eyes.

ranged in such a critical system, we find that the Renyi entropy still exhibit a linear scaling with boundary length in the thermodynamic limit if we consider separately the Renyi entropy of even and odd sized subsystems. No logarithmic correction to the scaling is found.

The power of this new algorithm is of course not limited to the above demonstrations. As QDM now becomes an important playground for the construction and detection of novel quantum state of matter[1], it is interesting to apply the new algorithm to more general QDM systems. In this respect, it is particularly interesting to study QDM defined on three dimensional lattice and to see how the ideas for 2D systems can be generalized to 3D system and what kind of new structure can emerge. As an concrete example, QDM defined on the pyrochlore lattice is especially attractive since it is closely related to the Kagome lattice quantum spin liquid on the one hand[20] and to the spin ice and monopole excitation on the other hand[21].

After the completion of this work, we notice a recent work on the evaluation of the Renyi entanglement entropy of QDM at the R-K point[22]. In their work, a ratio estimator trick first proposed in the study of spinful RVB state[18] is adopted. This trick, working like peeling the onion, involves the calculation of the ratios of REE on a serials of subsystems with decreasing sizes. Our algorithm, on the other hand, only involves the evaluation of the REE at a fixed subsystem size and is thus much easier to implement for more complex models.

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Note: Qiang Han is now an undergraduate student of the department and should not to be mistaken as the professor in the department with the same name.

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